STN - Structure Search 9/29/06

10/566,252

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Inventors

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:120883 CAPLUS
DOCUMENT NUMBER: 142:219153
TITLE: Preparation of (piperidylalkyl)benzylamine derivatives as tachykinin receptors antagonists
INVENTOR(S): Nagasawa, Masaaki; Kawase, Nobuo; Tanaka, Nobuyuki; Nakamura, Hideki; Tsuzuike, Naoki; Murata, Masakazu
PATENT ASSIGNEE(S): Zeria Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 248 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005012248 | A1 | 20050210 | WO 2004-JP11065 | 20040802 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2004261534 | A1 | 20050210 | AU 2004-261534 | 20040802 |
| CA 2534460 | AA | 20050210 | CA 2004-2534460 | 20040802 |
| EP 1650189 | A1 | 20060426 | EP 2004-748198 | 20040802 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK | | | | |
| CN 1829689 | A | 20060906 | CN 2004-80021890 | 20040802 |
| US 2006194841 | A1 | 20060831 | US 2006-566252 | 20060130 |
| PRIORITY APPLN. INFO.: | | | JP 2003-205114 A | 20030731 |
| | | | WO 2004-JP11065 W | 20040802 |

OTHER SOURCE(S): MARPAT 142:219153
GI

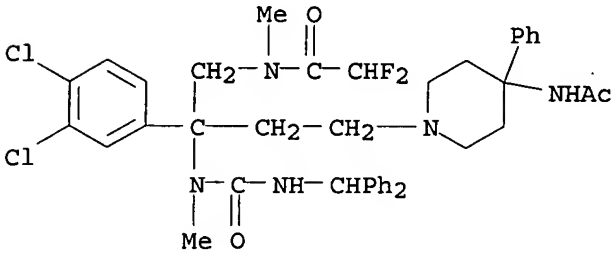
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [wherein X1 = NMe, NH, or O; X2 = a single bond, NH, CONH, O, S, etc.; X3 and X4 = independently H or halo; R1 = H, alkyl, (un)substituted Ph, etc.; R2 = H, alkyl, alkenyl, etc.; R3 = alkanoylamino, aminoalkanoyl, aminoalkanoylamino, etc.; R4 = H or forming a ring with R3; R5 = H or alkyl; m = 1 or 2; n = 0 or 1] or salts thereof are prepared as tachykinin receptors (NK) antagonists. For example, the compound II was prepared in a multi-step synthesis. II showed antagonistic activity with IC50 of 0.9 nM against human NK1. I are useful for the treatment of irritable bowel syndrome, pain, anxiety, obstructive bronchial diseases, headache, and vomiting (no data).

IT 841255-89-8P 841255-92-3P 841255-93-4P
841255-94-5P 841255-95-6P 841255-96-7P
841255-97-8P 841256-39-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(drug candidate; preparation of (piperidylalkyl)benzylamine derivs. as tachykinin receptors antagonists)

RN 841255-89-8 CAPLUS
CN Acetamide, N-[4-[4-(acetylamino)-4-phenyl-1-piperidinyl]-2-(3,4-dichlorophenyl)-2-[[[(diphenylmethyl)amino]carbonyl]methylamino]butyl]-2,2-difluoro-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



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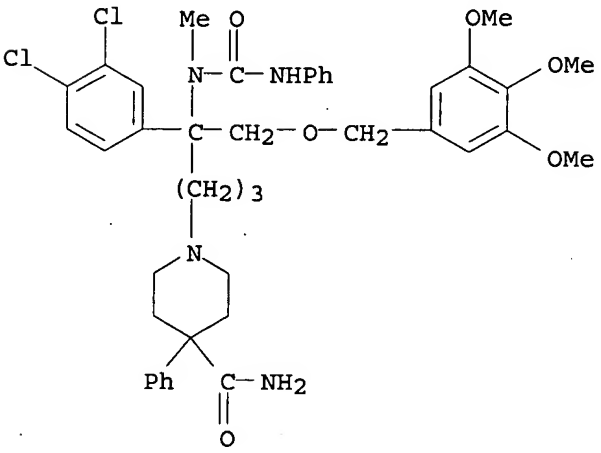
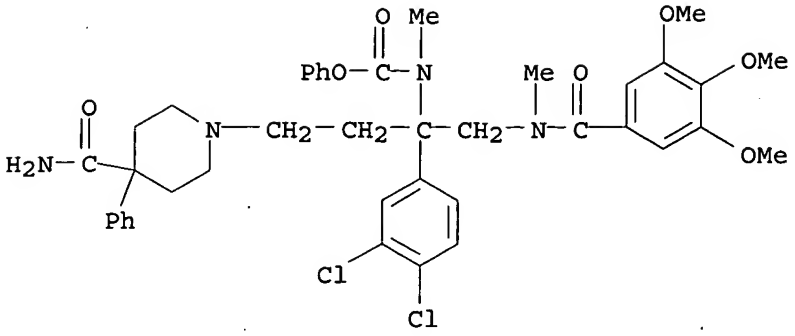
RN 841255-92-3 CAPLUS
CN 4-Piperidinecarboxamide, 1-[4-(3,4-dichlorophenyl)-4-[methyl[(phenylamino)carbonyl]amino]-5-[(3,4,5-trimethoxyphenyl)methoxy]pentyl]-4-phenyl- (9CI) (CA INDEX NAME)

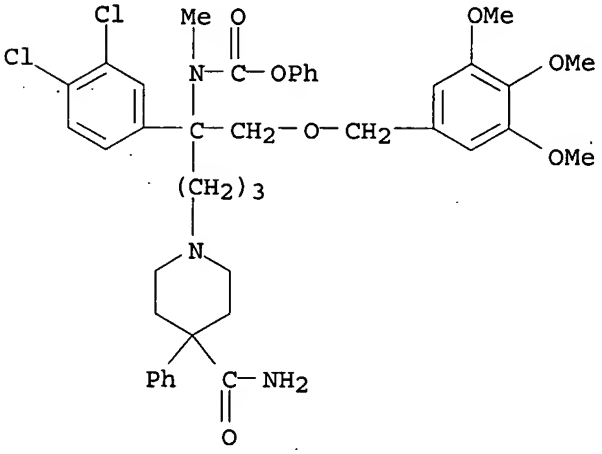


RN 841255-93-4 CAPLUS
CN Carbamic acid, [3-[4-(aminocarbonyl)-4-phenyl-1-piperidinyl]-1-(3,4-dichlorophenyl)-1-[[methyl(3,4,5-trimethoxybenzoyl)amino]methyl]propyl]methyl-, phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



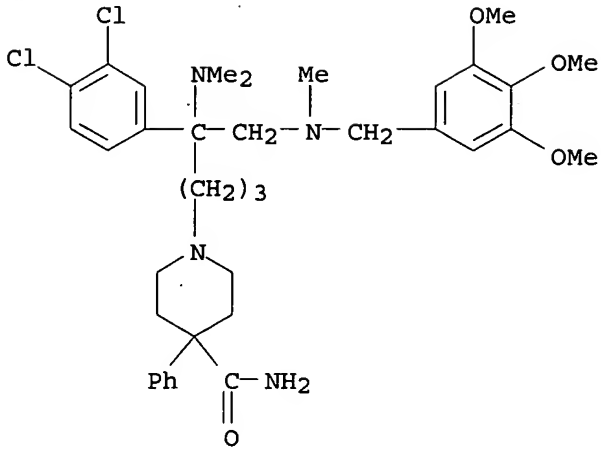
● HCl

RN 841255-94-5 CAPLUS
CN Carbamic acid, [4-[4-(aminocarbonyl)-4-phenyl-1-piperidinyl]-1-(3,4-dichlorophenyl)-1-[[(3,4,5-trimethoxyphenyl)methoxy]methyl]butyl]methyl-, phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

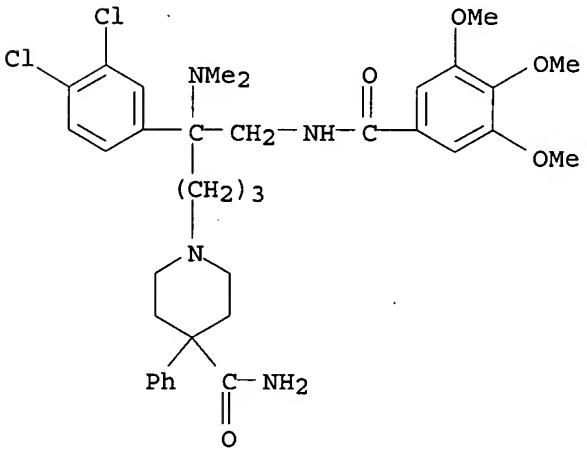


● HCl

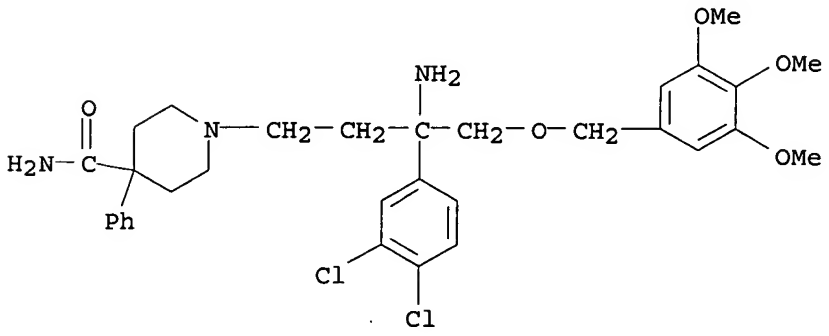
RN 841255-95-6 CAPLUS
CN 4-Piperidinecarboxamide, 1-[4-(3,4-dichlorophenyl)-4-(dimethylamino)-5-[methyl[(3,4,5-trimethoxyphenyl)methyl]amino]pentyl]-4-phenyl- (9CI) (CA INDEX NAME)



RN 841255-96-7 CAPLUS
CN 4-Piperidinecarboxamide, 1-[4-(3,4-dichlorophenyl)-4-(dimethylamino)-5-[(3,4,5-trimethoxybenzoyl)amino]pentyl]-4-phenyl- (9CI) (CA INDEX NAME)



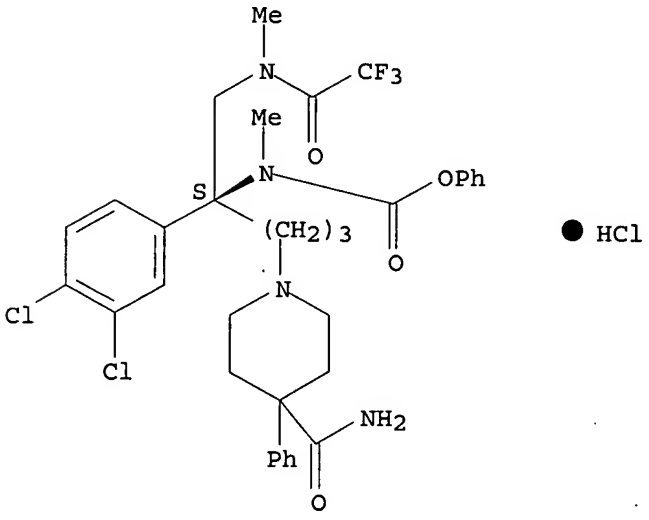
RN 841255-97-8 CAPLUS
CN 4-Piperidinecarboxamide, 1-[3-amino-3-(3,4-dichlorophenyl)-4-[(3,4,5-trimethoxyphenyl)methoxy]butyl]-4-phenyl- (9CI) (CA INDEX NAME)



RN 841256-39-1 CAPLUS
CN Carbamic acid, [(1S)-4-[4-(aminocarbonyl)-4-phenyl-1-piperidinyl]-1-(3,4-

dichlorophenyl)-1-[[methyl(trifluoroacetyl)amino]methyl]butyl]methyl-, phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

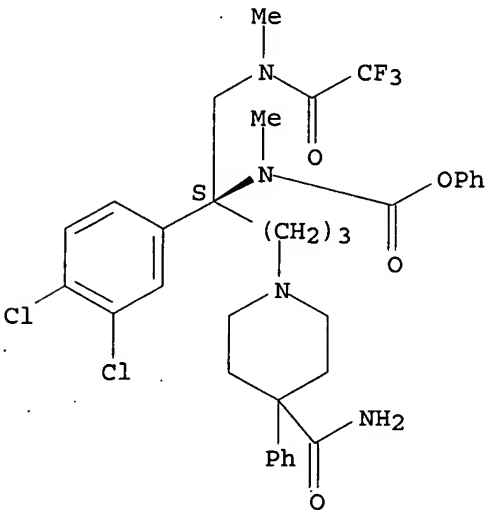


IT 841257-84-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (piperidylalkyl)benzylamine derivs. as tachykinin receptors antagonists)

RN 841257-84-9 CAPLUS

CN Carbamic acid, [(1S)-4-[4-(aminocarbonyl)-4-phenyl-1-piperidinyl]-1-(3,4-dichlorophenyl)-1-[[methyl(trifluoroacetyl)amino]methyl]butyl]methyl-, phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2006 ACS on STN
RE
(1) Astra Zeneca Ab; WO 0002859 A1 2002 CAPLUS
(2) Astra Zeneca Ab; EP 1097137 A1 2002 CAPLUS
(3) Astra Zeneca Ab; CN 1309638 A 2002
(4) Astra Zeneca Ab; CN 1322134 A 2002
(5) Astra Zeneca Ab; MX 2001000268 A 2002
(6) Astra Zeneca Ab; ZA 200100032 A 2002
(7) Astra Zeneca Ab; NO 200100151 A 2002
(8) Astra Zeneca Ab; MX 2001003560 A 2002
(9) Astra Zeneca Ab; ZA 200102651 A 2002
(10) Astra Zeneca Ab; ZA 200102658 A 2002
(11) Astra Zeneca Ab; KR 2001083100 A 2002
(12) Astra Zeneca Ab; JP 2002520316 A 2002
(13) Astra Zeneca Ab; US 6365602 B1 2002 CAPLUS
(14) Astra Zeneca Ab; BR 9912013 A 2002 CAPLUS
(15) Astra Zeneca Ab; BR 9914333 A 2002 CAPLUS
(16) Astra Zeneca Ab; AU 9946378 A 2002 CAPLUS
(17) Merck & Co Inc; JP 08-505880 A 1996
(18) Merck & Co Inc; JP 08-511522 A 1996
(19) Merck & Co Inc; US 5869496 A 1996 CAPLUS
(20) Merck & Co Inc; US 6013652 A 1996 CAPLUS
(21) Merck & Co Inc; EP 681571 A1 1996 CAPLUS
(22) Merck & Co Inc; EP 702681 A1 1996 CAPLUS
(23) Merck & Co Inc; ZA 9403946 A 1996 CAPLUS
(24) Merck & Co Inc; WO 9417045 A1 1996 CAPLUS
(25) Merck & Co Inc; WO 9429309 A1 1996 CAPLUS
(26) Merck & Co Inc; AU 9461268 A 1996 CAPLUS
(27) Merck & Co Inc; AU 9472011 A 1996 CAPLUS
(28) Schering Corp; US 5789422 A 1998 CAPLUS
(29) Schering Corp; KR 2000052856 A 2001 CAPLUS
(30) Schering Corp; JP 2001507673 A 2001
(31) Schering Corp; NZ 334966 A 2001 CAPLUS
(32) Schering Corp; EP 934271 A1 2001 CAPLUS
(33) Schering Corp; AU 9674607 A 2001 CAPLUS
(34) Schering Corp; WO 9818761 A1 2001 CAPLUS
(35) Schering Corp; HU 9903653 A 2001
(36) Schering Corp; MX 9903894 A 2001


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L3          12 S L1 FULL

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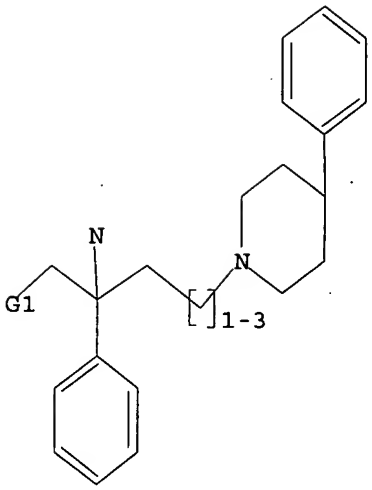


G1 O,N

Structure attributes must be viewed using STN Express query preparation.

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L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:120883 CAPLUS
DOCUMENT NUMBER: 142:219153
TITLE: Preparation of (piperidylalkyl)benzylamine derivatives as tachykinin receptors antagonists
INVENTOR(S): Nagasawa, Masaaki; Kawase, Nobuo; Tanaka, Nobuyuki; Nakamura, Hideki; Tsuzuike, Naoki; Murata, Masakazu
PATENT ASSIGNEE(S): Zeria Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 248 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005012248 | A1 | 20050210 | WO 2004-JP11065 | 20040802 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
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| EP 1650189 | A1 | 20060426 | EP 2004-748198 | 20040802 |
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| CN 1829689 | A | 20060906 | CN 2004-80021890 | 20040802 |

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| US 2006194841 | A1 | 20060831 | US 2006-566252 | | 20060130 |
| PRIORITY APPLN. INFO.: | | | JP 2003-205114 | A | 20030731 |
| | | | WO 2004-JP11065 | W | 20040802 |

OTHER SOURCE(S): MARPAT 142:219153
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [wherein X1 = NMe, NH, or O; X2 = a single bond, NH, CONH, O, S, etc.; X3 and X4 = independently H or halo; R1 = H, alkyl, (un)substituted Ph, etc.; R2 = H, alkyl, alkenyl, etc.; R3 = alkanoylamino, aminoalkanoyl, aminoalkanoylamino, etc.; R4 = H or forming a ring with R3; R5 = H or alkyl; m = 1 or 2; n = 0 or 1] or salts thereof are prepared as tachykinin receptors (NK) antagonists. For example, the compound II was prepared in a multi-step synthesis. II showed antagonistic activity with IC50 of 0.9 nM against human NK1. I are useful for the treatment of irritable bowel syndrome, pain, anxiety, obstructive bronchial diseases, headache, and vomiting (no data).

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=> d his

(FILE 'HOME' ENTERED AT 11:23:50 ON 29 SEP 2006)

FILE 'REGISTRY' ENTERED AT 11:24:28 ON 29 SEP 2006
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 12 S L1 FULL

FILE 'CAPLUS' ENTERED AT 11:25:02 ON 29 SEP 2006
L4 1 S L3

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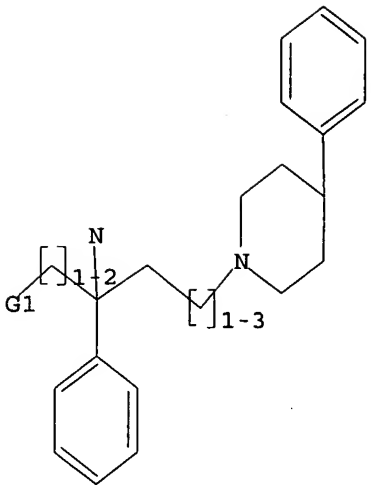


G1 O,N

Structure attributes must be viewed using STN Express query preparation.

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